

Supporting information file

Synthesis, Characterization and Multi Dimensional Application Approach of Two Distinctive Tetra Nuclear First Time Reported Fe³⁺/Hg²⁺ and Fe³⁺/Cd²⁺ clusters from a New Fe³⁺ Containing Metalloligand

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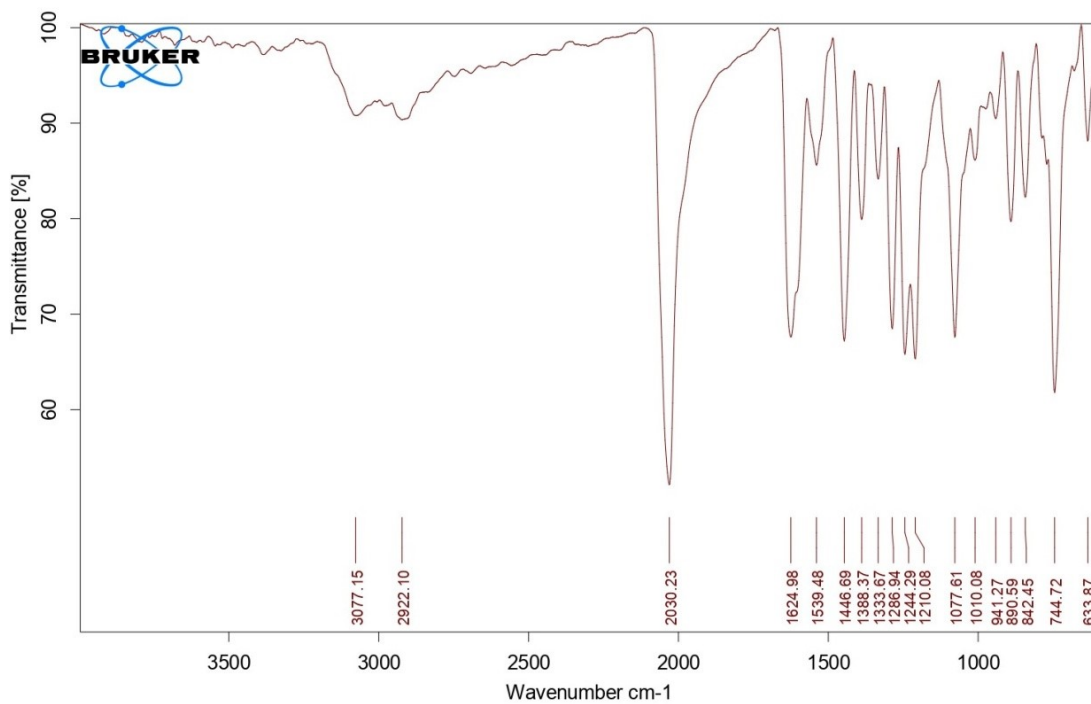


Fig. S1 FTIR spectrum of MC1

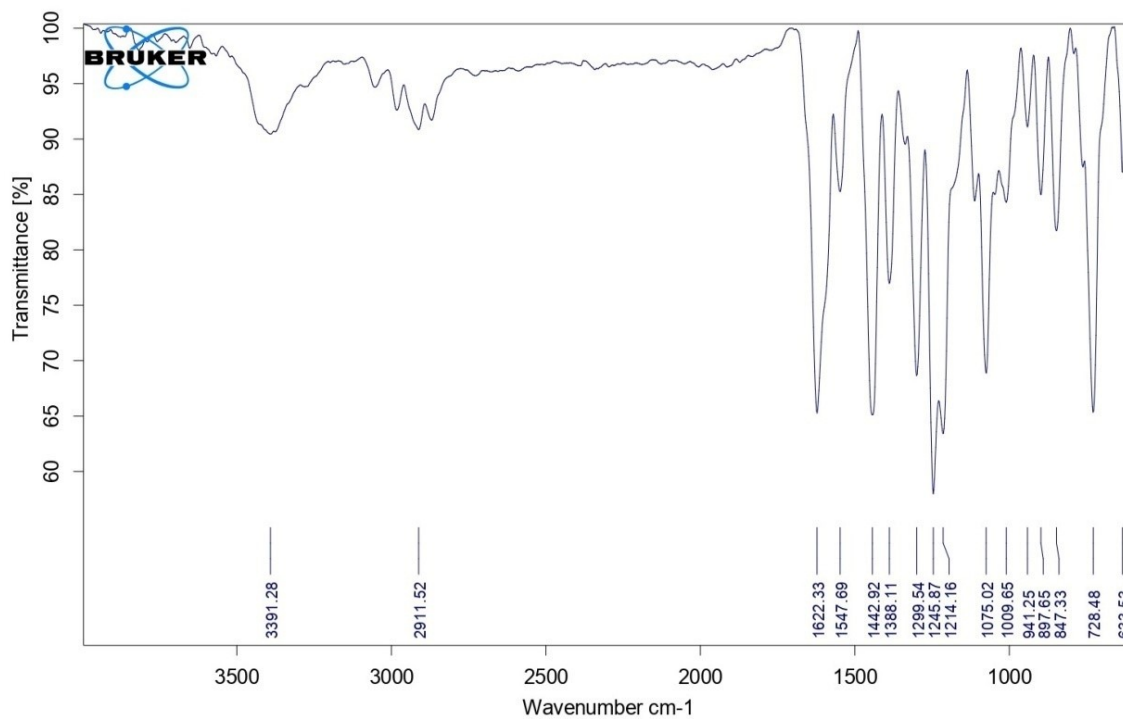


Fig. S2: FTIR spectrum of MC2

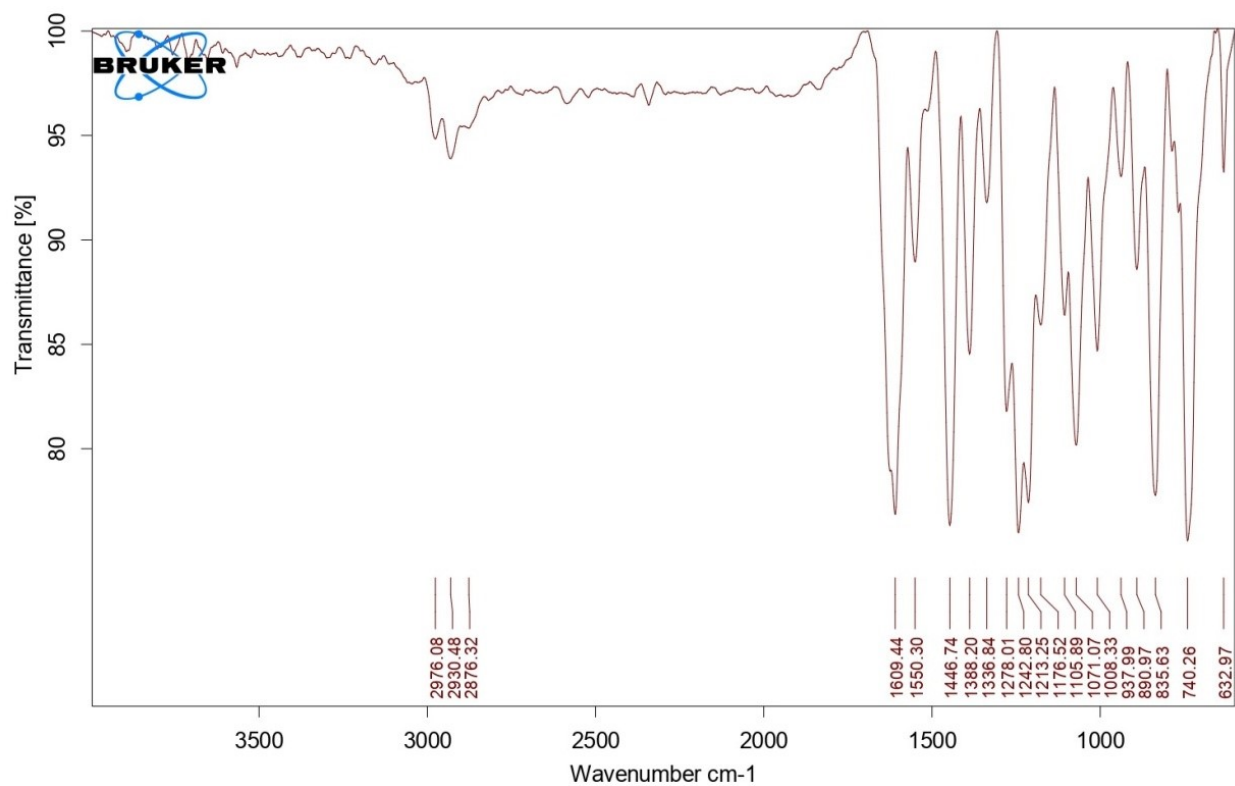


Fig. S3: FTIR spectrum of MC3

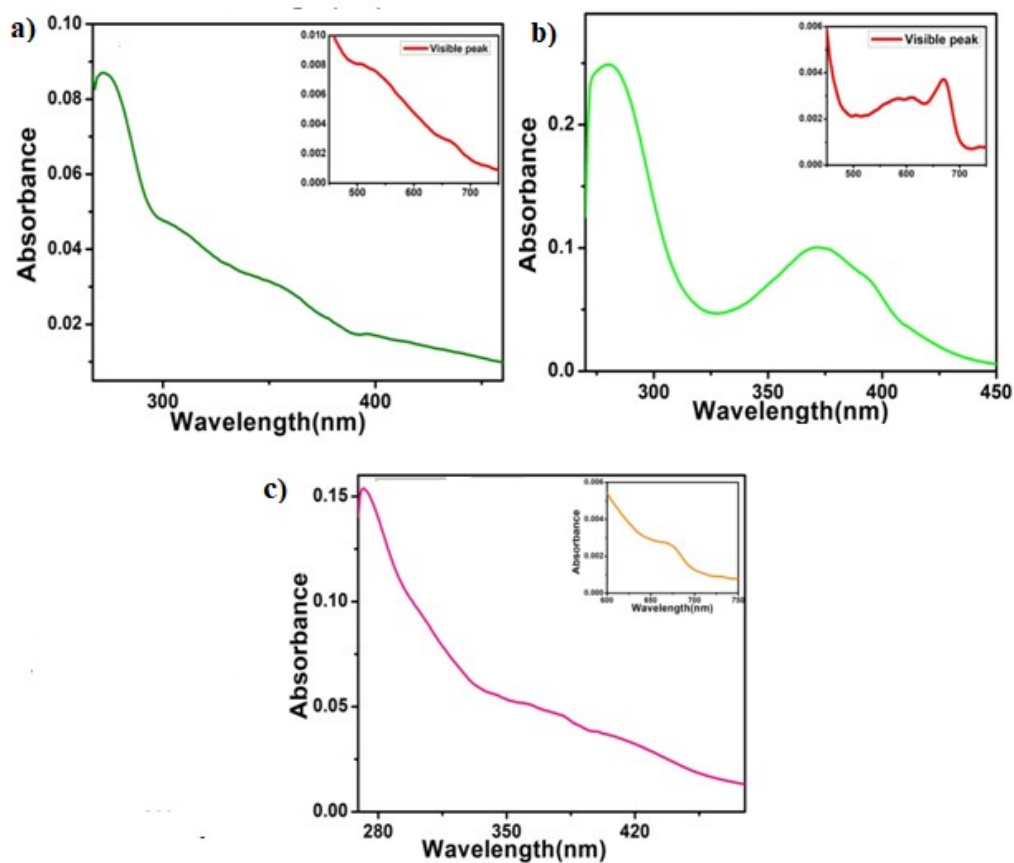


Fig. S4: UV spectrum a) MC1 b) MC2 c) MC3

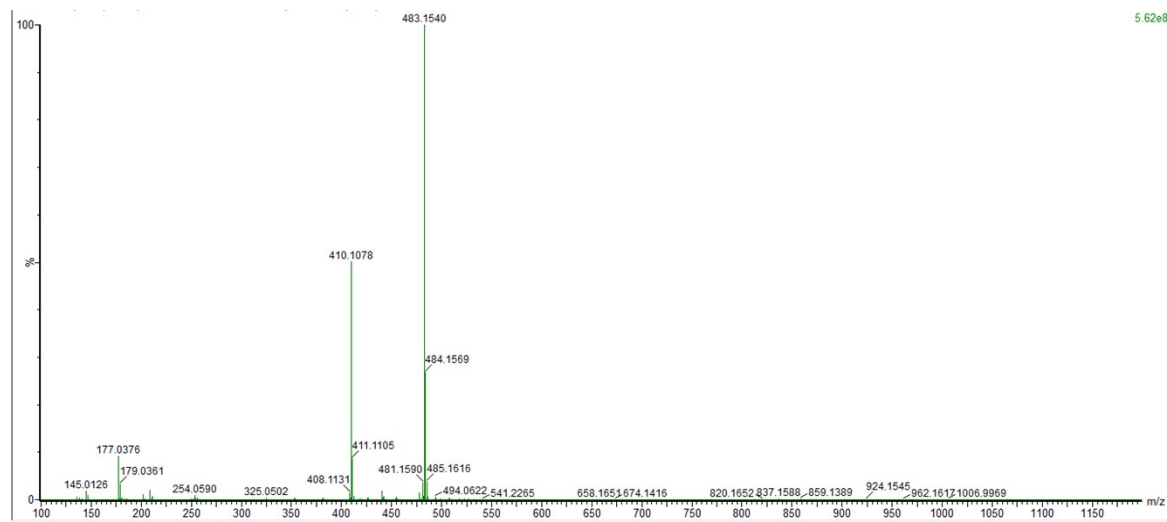
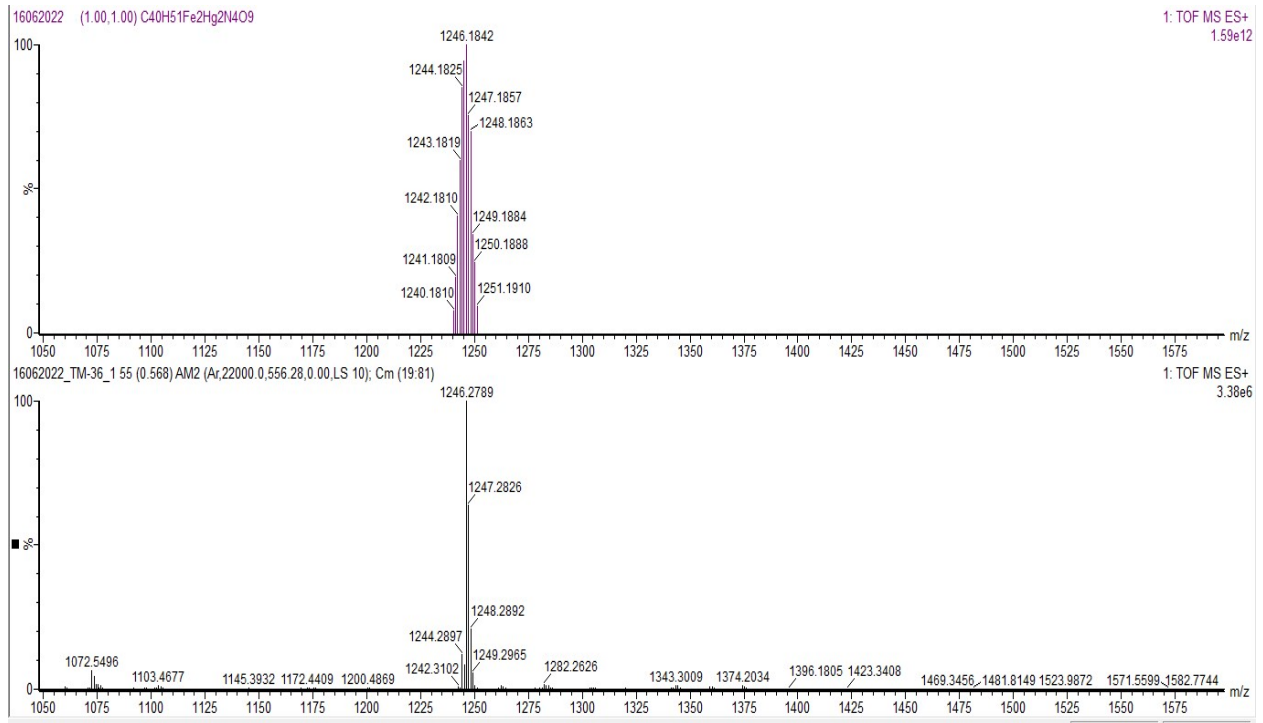


Fig. S5 Mass spectra of MC1

a)



b)

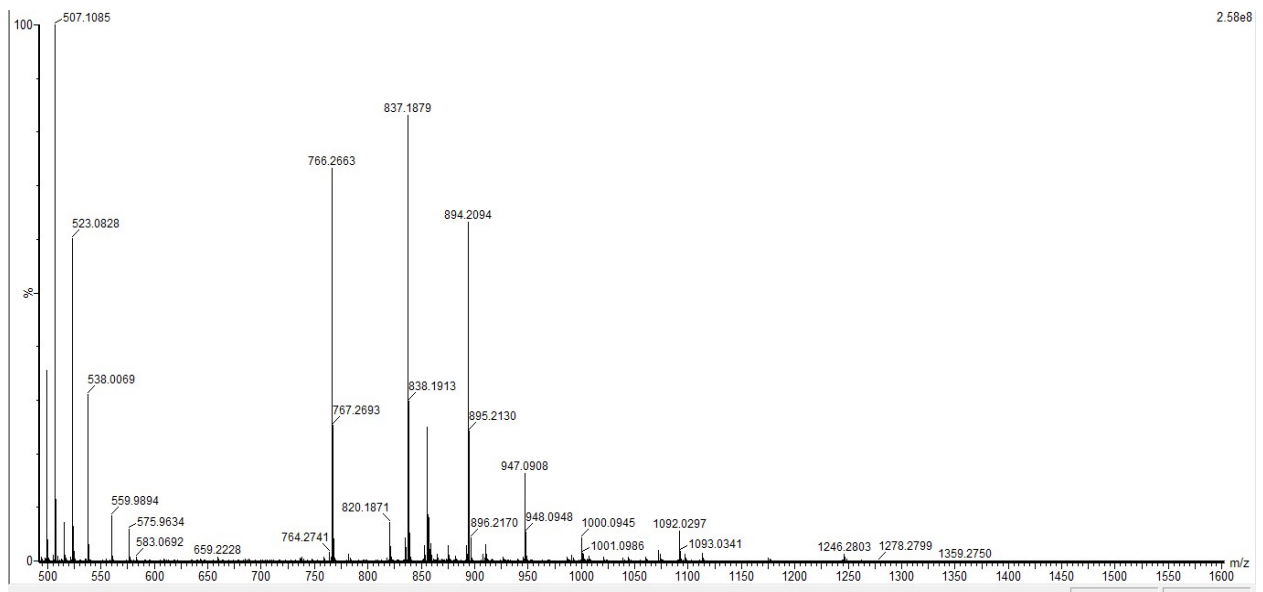


Fig. S6 Mass spectra of a) MC2 b) MC4

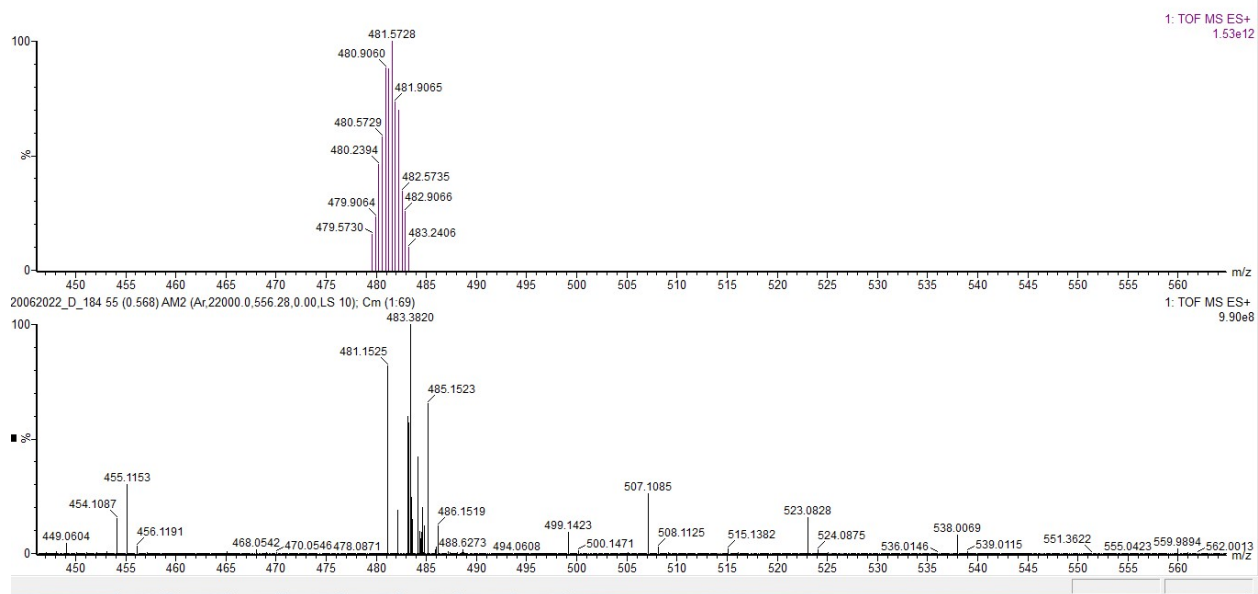


Fig. S7 Mass spectra of MC3

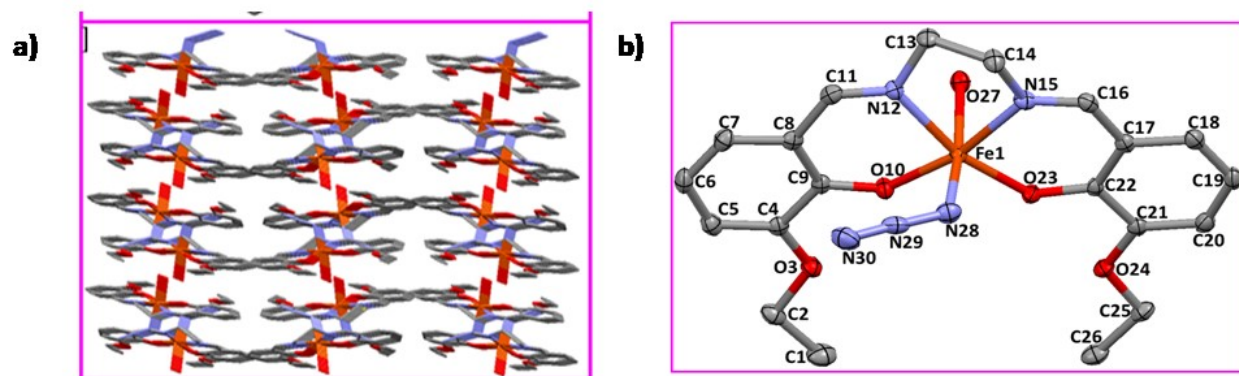


Fig. S8: a) The overall packing of the crystal structure b) Molecular plot of MC1

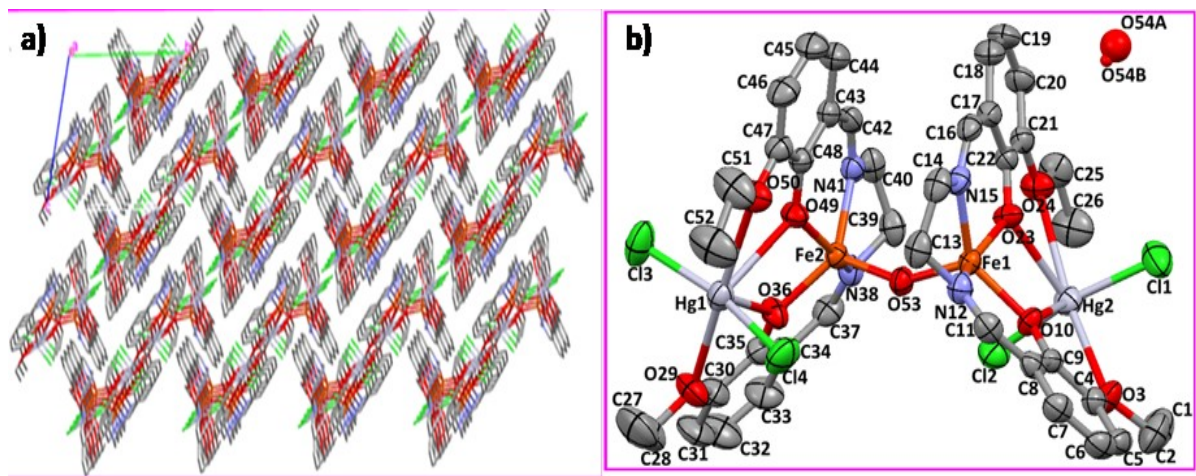


Fig. S9: a) The overall packing of the crystal structure b) Molecular plot of MC2

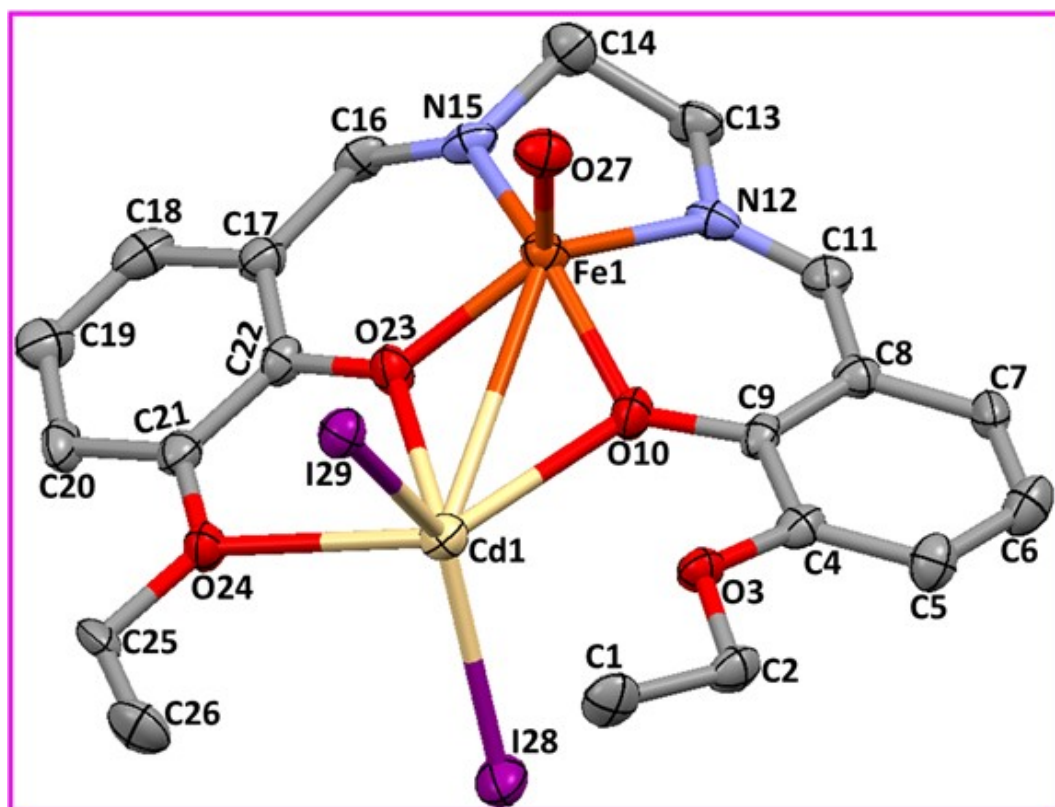


Fig. S10: Molecular plot of MC3

Table S1: Hydrogen bonding parameter of MC1

D-H...A	D-H (Å)	H...A (Å)	D...A (Å)	D-H...A (°)	Symmetry operation for A
O(27)–H(27A)•••O23	0.804	2.199	2.965	159.47	-x+1, -y+1, -z+1
O(27)–H(27B)•••O10	0.674	2.252	2.835	145.73	-x+1, -y+1, -z+1

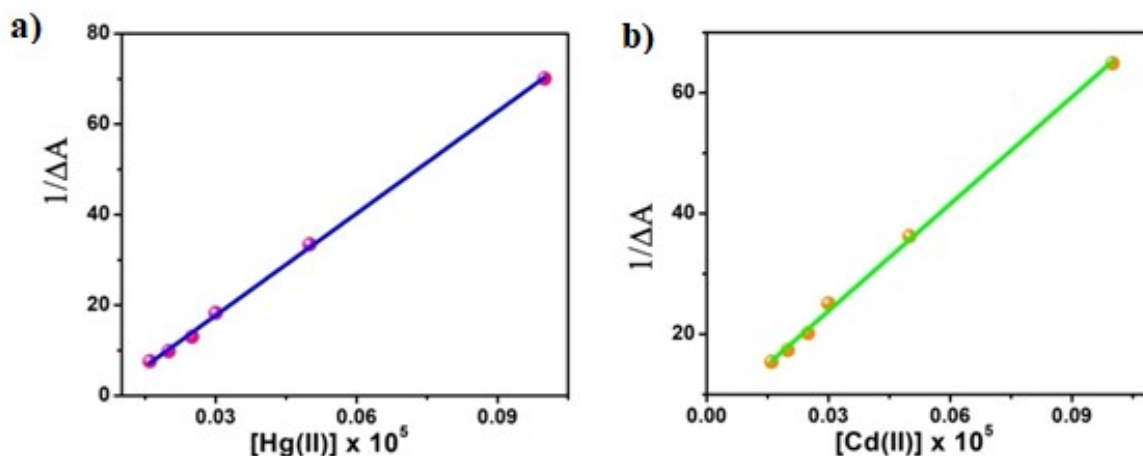


Fig. S11: Binding constant determination of a) MC1-Hg(II) adduct c) MC1-Cd(II) adduct

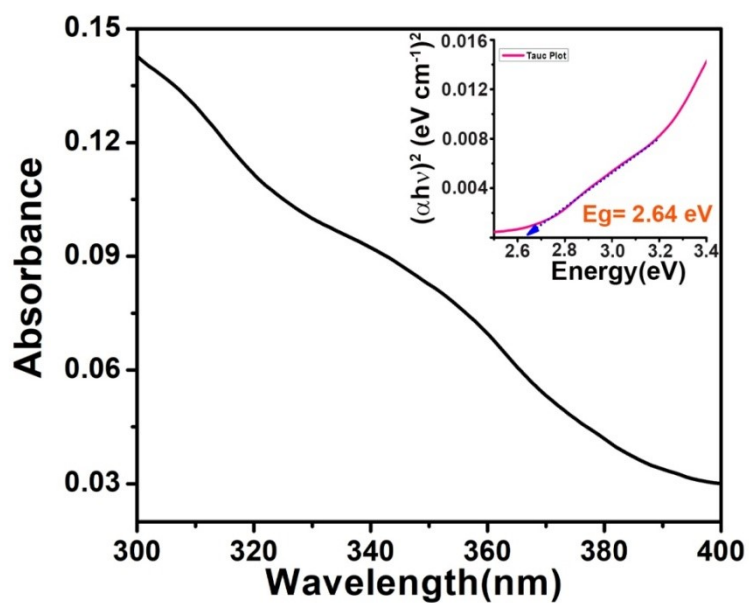


Fig. S12: Band gap calculation of MC4

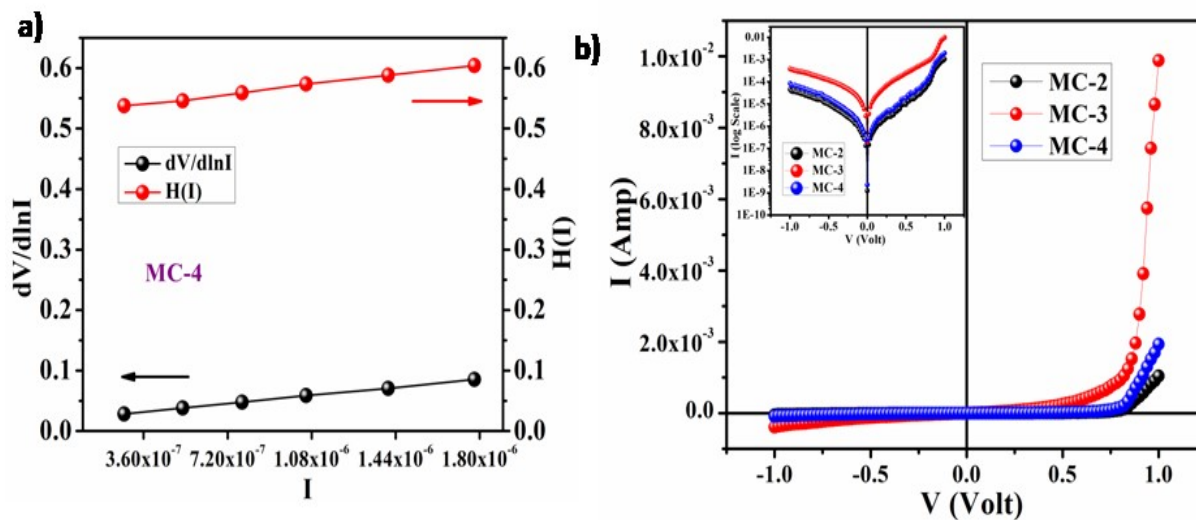


Fig. S13 a) $dV/d\ln I$ vs. I and $H(I)$ vs. I curves for device-C b) Current-voltage characteristics plot for device A, B, C under dark condition and $\log I$ vs V plot for device A, B and C.

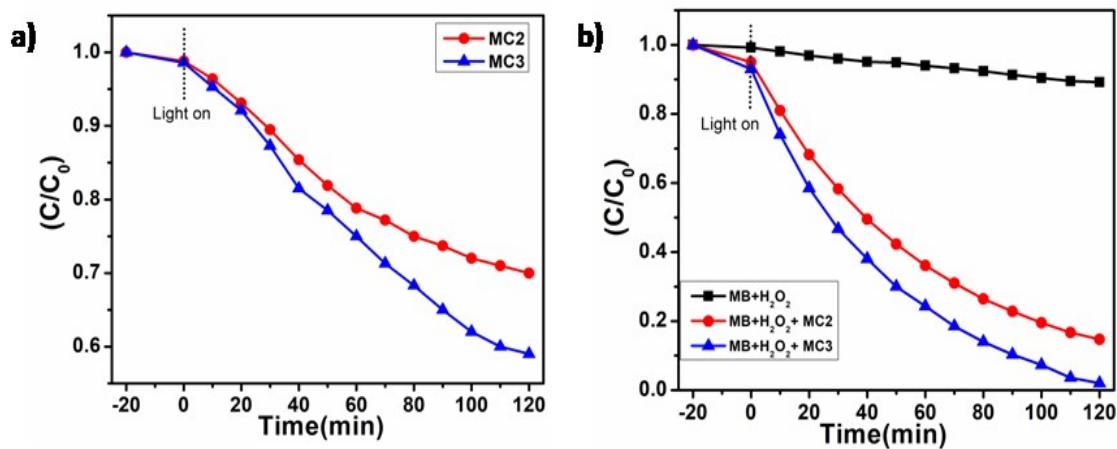


Fig. S14: Rate of methylene blue degradation in presence of a) only complex b) complex in presence of H_2O_2 .

Table S2: Photocatalytic Methylene blue dye degradation rate constant by changing the different parameter

Sample composition	Rate constant in min^{-1} of MB dye degradation	pH values	Rate constant in min^{-1} of MB dye degradation by MC3 catalysis	Stoichiometry change of MC3 catalyst	Rate constant in min^{-1}
Only in presence of H_2O_2	0.0015	3	0.0034	10 mg of MC3	0.015
H_2O_2 + MC2	0.0156(10 times)	7	.009	20 mg of MC3	0.256
H_2O_2 + MC3	0.0259(17 times)	9	.010		
		11	.013	30 mg of MC3	0.272

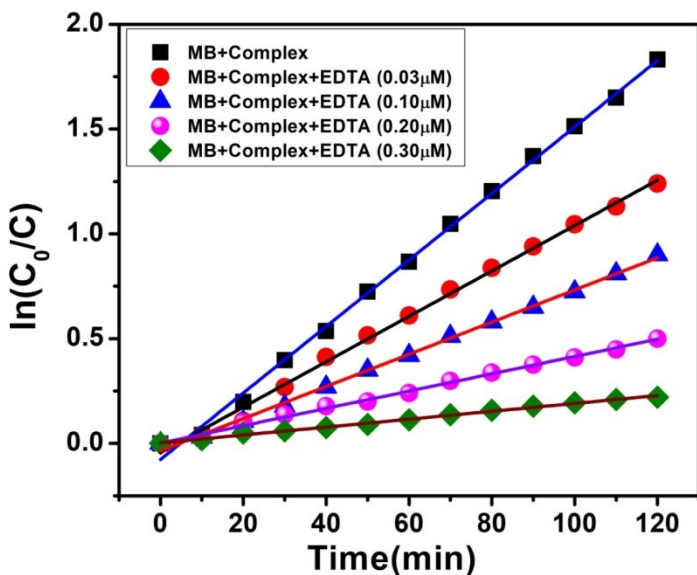


Fig. S15: Plot of $\ln(C_0/C)$ vs time for the pseudo first order kinetics curves of the photocatalytic degradation of methylene blue by using **MC3** catalyst in presence of stoichiometric inhibitor EDTA